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Microscopic collective dynamics of water

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Abstract

© 2016, Pleiades Publishing, Ltd.Data obtained on microscopic collective excitations in water by molecular dynamics simulation within the framework of the coarse-grained mW-model of the intermolecular interaction potential for water are reported. The calculated spectra of the dynamic structure factor and spectral densities of time correlation functions of longitudinal and transverse currents reveal the existence of propagating collective excitations of longitudinal and transverse polarization in water for a wide range of wavenumbers. The dynamics of fluctuations in the particle number density is analyzed within the framework of a microscopic theory that takes into account only the structural features of a system. The theoretically calculated data on the spectra of dynamic structure factor in a wavenumber range of 0.13–0.48 Å–1 are in good agreement with the results of molecular dynamics simulation.

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